Mathmatial Foundations of Reinforcement Learning

Policy optimization: REINFORCE, PG and NPG

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Outline

Introduction to policy gradient methods

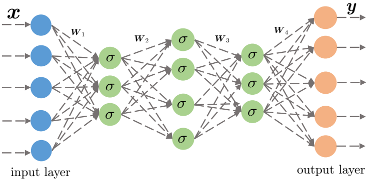
Global convergence of softmax policy gradient methods

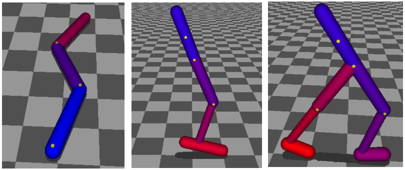
Natural policy gradient methods

Policy optimization

$$\text{maximize}_\theta \quad \text{value}(\text{policy}(\theta))$$

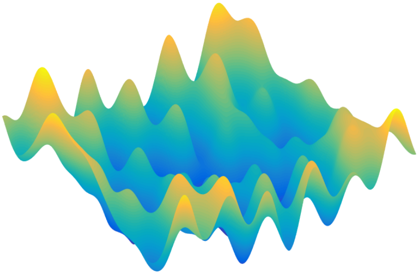
- directly optimize the policy, which is the quantity of interest;
- allow flexible differentiable parameterizations of the policy;
- work with both continuous and discrete problems.





Theoretical challenges: non-concavity

Little understanding on the global convergence of policy gradient methods until very recently, e.g. (Fazel et al., 2018; Bhandari and Russo, 2019; Agarwal et al., 2019; Mei et al. 2020), and many more.



Our goal:

- introduce the algorithmic framework of popular policy gradient methods
- understand finite-time convergence rates of popular heuristics

Introduction to policy gradient methods

Policy gradient methods

Given an initial state distribution $s \sim \rho$, find policy π such that

$$\text{maximize}_{\pi} \quad V^{\pi}(\rho) := \mathbb{E}_{s\sim\rho}\left[V^{\pi}(s)\right]$$

$$\Downarrow$$

Parameterization:
$$\pi := \pi_\theta$$

$$\text{maximize}_{\theta} \quad V^{\pi_\theta}(\rho) := \mathbb{E}_{s\sim\rho}\left[V^{\pi_\theta}(s)\right]$$

Policy gradient method

For $t = 0, 1, \cdots$

$$\theta^{(t+1)} = \theta^{(t)} + \eta \nabla_\theta V^{\pi_\theta^{(t)}}(\rho)$$

where η *is the learning rate.*

How to calculate the gradient?

Policy gradient derivation

- Assume π_θ is differentiable when it is non-zero with gradient $\nabla_\theta \pi_\theta$.

The policy gradient can be decomposed as

$$
\begin{aligned}
&\nabla_\theta V^{\pi_\theta}(\rho) \\
&= \nabla_\theta \mathbb{E}_{s_0 \sim \rho}\left[V^{\pi_\theta}(s_0)\right] \\
&= \mathbb{E}_{s_0 \sim \rho}\left[\nabla_\theta \left(\sum_{a_0 \in \mathcal{A}} \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0)\right)\right] \\
&= \mathbb{E}_{s_0 \sim \rho}\left[\sum_{a_0 \in \mathcal{A}} \nabla_\theta \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) + \sum_{a_0 \in \mathcal{A}} \pi_\theta(a_0|s_0) \nabla_\theta Q^{\pi_\theta}(s_0, a_0)\right]
\end{aligned}
$$

We discuss the two terms separately.

Policy gradient derivation - first term

Note that

$$\nabla_\theta \pi_\theta(a|s) = \pi_\theta(a|s) \frac{\nabla_\theta \pi_\theta(a|s)}{\pi_\theta(a|s)} = \pi_\theta(a|s) \underbrace{\nabla_\theta \log \pi_\theta(a|s)}_{\text{score function}}.$$

The first term in the policy gradient is expressed as

$$\begin{aligned}
&\mathbb{E}_{s_0 \sim \rho} \left[\sum_{a_0 \in \mathcal{A}} \nabla_\theta \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) \right] \\
&= \mathbb{E}_{s_0 \sim \rho} \left[\sum_{a_0 \in \mathcal{A}} \pi_\theta(a_0|s_0) \nabla_\theta \log \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) \right] \\
&= \mathbb{E}_{s_0 \sim \rho, a_0 \sim \pi_\theta(\cdot|s_0)} \left[\nabla_\theta \log \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0, a_0) \right]
\end{aligned}$$

Policy gradient derivation - second term

The second term in the policy gradient is expressed as

$$
\begin{aligned}
&\mathbb{E}_{s_0\sim\rho}\left[\sum_{a_0\in\mathcal{A}} \pi_\theta(a_0|s_0)\nabla_\theta Q^{\pi_\theta}(s_0,a_0)\right] \\
&= \mathbb{E}_{s_0\sim\rho, a_0\sim\pi_\theta(\cdot|s_0)}\big[\nabla_\theta Q^{\pi_\theta}(s_0,a_0)\big] \\
&= \mathbb{E}_{s_0\sim\rho, a_0\sim\pi_\theta(\cdot|s_0)}\,\Big[\nabla_\theta\big(r(s_0,a_0)+\gamma\mathbb{E}_{s_1\sim P(\cdot|s_0,a_0)}V^{\pi_\theta}(s_1)\big)\Big] \\
&= \gamma\mathbb{E}_{s_0\sim\rho, a_0\sim\pi_\theta(\cdot|s_0), s_1\sim P(\cdot|s_0,a_0)}\big[\nabla_\theta V^{\pi_\theta}(s_1)\big],
\end{aligned}
$$

which is similar to what we want to bound, but a discounted one-step look-ahead.

Policy gradient derivation - recursion

Letting τ denote the trajectory following policy π_θ, by recursion,

$$\begin{aligned}
\nabla_\theta V^{\pi_\theta}(\rho) &= \mathbb{E}_{s_0\sim\rho, a_0\sim\pi_\theta(\cdot|s_0)}\left[\nabla_\theta \log \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0,a_0)\right] \\
&\qquad + \gamma \mathbb{E}_{s_0\sim\rho, a_0\sim\pi_\theta(\cdot|s_0), s_1\sim P(\cdot|s_0,a_0)}\left[\nabla_\theta V^{\pi_\theta}(s_1)\right] \\
&= \mathbb{E}_{(s_0,a_0)\sim\tau}\left[\nabla_\theta \log \pi_\theta(a_0|s_0) Q^{\pi_\theta}(s_0,a_0)\right] \\
&\qquad + \gamma \mathbb{E}_{(s_0,a_0,s_1,a_1)\sim\tau}\left[\nabla_\theta \log \pi_\theta(a_1|s_1) Q^{\pi_\theta}(s_1,a_1)\right] + \dots \\
&= \mathbb{E}_{(s_i,a_i)_{i\geq 0}\sim\tau}\left[\sum_{i=0}^{\infty} \gamma^t \nabla_\theta \log \pi_\theta(a_i|s_i) Q^{\pi_\theta}(s_i,a_i)\right] \\
&= \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\rho^{\pi_\theta}, a\sim\pi_\theta(\cdot|s)}\Big[Q^{\pi_\theta}(s,a)\nabla \log \pi_\theta(a|s)\Big],
\end{aligned}$$

where $d_\rho^{\pi_\theta}$ is the **state visitation distribution:**

$$d_{s_0}^{\pi}(s) = (1-\gamma)\sum_{t=0}^{\infty}\gamma^t \mathbb{P}^\pi(s_t = s \,|\, s_0), \qquad d_\rho^\pi = \mathbb{E}_{s_0\sim\rho}[d_{s_0}^\pi(s)].$$

The policy gradient theorem

Theorem 1 (Policy gradient theorem [Sutton et al., 1999])

The policy gradient can be evaluated via

$$\nabla_\theta V^{\pi_\theta}(\rho) = \frac{1}{1-\gamma} \mathbb{E}_{s \sim d_\rho^{\pi_\theta}, a \sim \pi_\theta(\cdot|s)} \Big[Q^{\pi_\theta}(s,a) \nabla \log \pi_\theta(a|s) \Big],$$

where

- $d_\rho^{\pi_\theta}$ *is the state visitation distribution,*
- $\nabla \log \pi_\theta(a|s)$ *is the score function.*

Provides an effective scheme for policy gradient evaluation (e.g., REINFORCE):

- rolling out trajectory following π_θ
- evaluating the value function Q^{π_θ}

Examples of policy parameterization

Discrete action space: softmax parameterization with function approximation

$$\pi_\theta(a|s) \propto \exp(\phi(s,a)^\top \theta)$$

- $\phi(s,a)$ is the feature vector of each state-action pair;
- the score function $\nabla \log \pi_\theta(a|s) = \phi(s,a) - \mathbb{E}_{a\sim\pi_\theta(\cdot|s)}[\phi(s,\cdot)]$.

Continuous action space: Gaussian policy

$$a \sim \mathcal{N}(\mu(s), \sigma^2), \quad \mu(s) = \phi(s)^\top \theta$$

- $\phi(s)$ is the feature of each state;
- σ^2 is the variance (kept constant for simplicity);
- the score function $\nabla \log \pi_\theta(a|s) = \frac{(a-\mu(s))\phi(s)}{\sigma^2}$.

Baseline

The policy gradient can have high variance with limited samples.

Variance reduction: introducing a baseline

$$\nabla_\theta V^{\pi_\theta}(\rho) = \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\rho^{\pi_\theta}, a\sim\pi_\theta(\cdot|s)}\Big[\left(Q^{\pi_\theta}(s,a) - b(s)\right)\nabla\log\pi_\theta(a|s)\Big],$$

to help minimize the variance:

$$\begin{aligned}
\mathbb{E}_{a\sim\pi_\theta(\cdot|s)}\Big[\nabla\log\pi_\theta(a|s)\Big] &= \sum_a \pi_\theta(a|s)\frac{\nabla_\theta\pi_\theta(a|s)}{\pi_\theta(a|s)} \\
&= \sum_a \nabla_\theta\pi_\theta(a|s) \\
&= \nabla_\theta \sum_a \pi_\theta(a|s) = 0
\end{aligned}$$

Baseline

Variance reduction: introducing a baseline

$$\nabla_\theta V^{\pi_\theta}(\rho) = \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\rho^{\pi_\theta}, a\sim\pi_\theta(\cdot|s)}\Big[\left(Q^{\pi_\theta}(s,a) - b(s)\right)\nabla\log\pi_\theta(a|s)\Big],$$

to help minimize the variance.

- In practice, choose $b(s) = V^{\pi_\theta}(s)$, leading to

$$\nabla_\theta V^{\pi_\theta}(\rho) = \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\rho^{\pi_\theta}, a\sim\pi_\theta(\cdot|s)}\Big[A^{\pi_\theta}(s,a)\nabla\log\pi_\theta(a|s)\Big]$$

- $A^\pi(s,a) = Q^\pi(s,a) - V^\pi(s)$ is the advantage function.
- Instead of estimating $Q^\pi(s,a)$, directly estimate $A^\pi(s,a)$.

Global convergence of softmax policy gradient methods

Softmax policy gradient methods

Given an initial state distribution $s \sim \rho$, find policy π such that

$$\text{maximize}_{\pi} \quad V^{\pi}(\rho) := \mathbb{E}_{s\sim\rho}\left[V^{\pi}(s)\right]$$

$$\Downarrow$$

softmax parameterization:
$$\pi_\theta(a|s) \propto \exp(\theta(s,a))$$

$$\text{maximize}_{\theta} \quad V^{\pi_\theta}(\rho) := \mathbb{E}_{s\sim\rho}\left[V^{\pi_\theta}(s)\right]$$

Policy gradient method

For $t = 0, 1, \cdots$

$$\theta^{(t+1)} = \theta^{(t)} + \eta \nabla_\theta V^{\pi_\theta^{(t)}}(\rho)$$

where η *is the learning rate.*

Global convergence of the PG method

Exact gradient evaluation: suppose we can perfectly evaluate the gradient

$$\nabla_\theta V^{\pi_\theta^{(t)}}(\rho),$$

does softmax policy gradient converge?

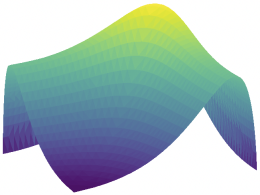
Theorem 2 ([Agarwal et al., 2021])

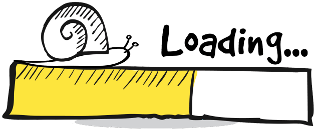
Assume ρ is strictly positive, i.e., $\rho(s) > 0$ for all states s. For $\eta \leq (1-\gamma)^3/8$, then we have that for all states s,

$$V^{(t)}(s) = V^{\pi_\theta^{(t)}}(s) \to V^\star(s), \qquad t \to \infty.$$

- Softmax policy gradient finds the global optimal policy despite conconcavity!

How fast does softmax PG converge?





- [Agarwal et al., 2021] showed that softmax PG converges asymptotically to the global optimal policy.
- [Mei et al., 2020] showed that softmax PG converges to global opt in

$$c\Big(|\mathcal{S}|, |\mathcal{A}|, \tfrac{1}{1-\gamma}, \cdots\Big)\, O\Big(\tfrac{1}{\varepsilon}\Big) \text{ iterations}$$

Is the rate of PG good, bad or ugly?

A negative message

Theorem 3 ([Li et al., 2023])

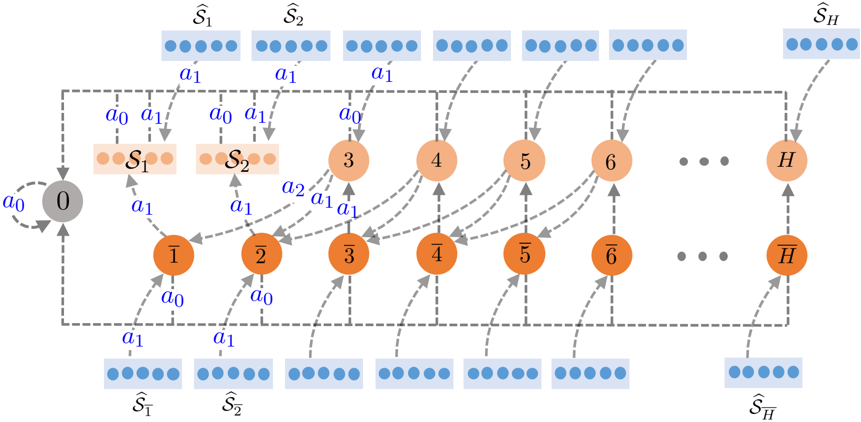
There exists an MDP s.t. it takes softmax PG at least

$$\frac{1}{\eta}|\mathcal{S}|^{2^{\Theta(\frac{1}{1-\gamma})}} \textit{ iterations}$$

to achieve $\|V^{(t)} - V^{\star}\|_{\infty} \leq 0.15$.

- Softmax PG can take (super)-exponential time to converge (in problems w/ large state space & long effective horizon)!
- Also hold for average sub-opt gap $\frac{1}{|\mathcal{S}|}\sum_{s\in\mathcal{S}}\left[V^{(t)}(s) - V^{\star}(s)\right]$.

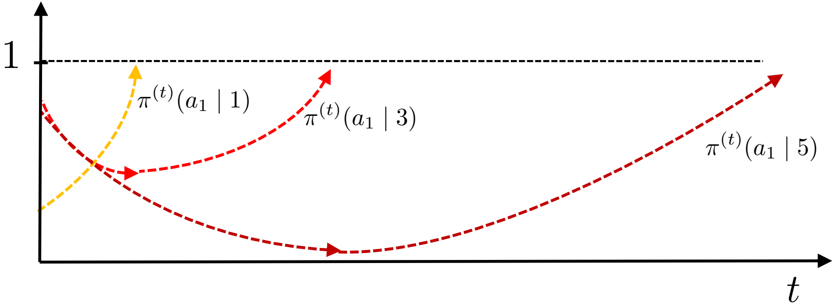
MDP construction for our lower bound



Key ingredients: for $3 \leq s \leq H \asymp \frac{1}{1-\gamma}$,

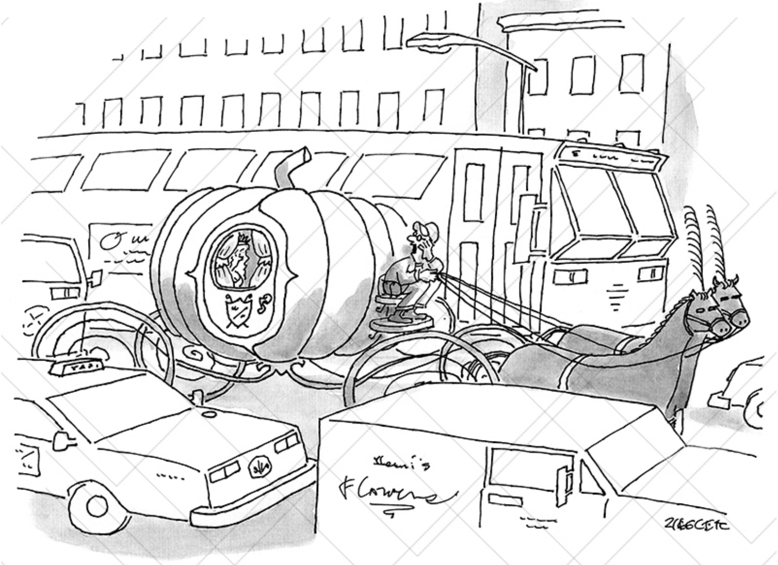
- $\pi^{(t)}(a_{\text{opt}} \mid s)$ keeps decreasing until $\pi^{(t)}(a_{\text{opt}} \mid s-2) \approx 1$

What is happening in our constructed MDP?



Convergence time for state s grows geometrically as s increases

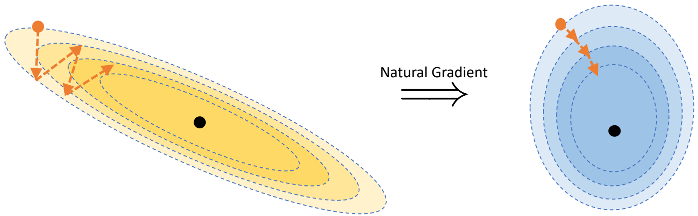
$$\text{convergence-time}(s) \gtrsim \big(\text{convergence-time}(s-2)\big)^{1.5}$$



"Seriously, lady, at this hour you'd make a lot better time taking the subway."

Natural policy gradient methods

Natural policy gradient



Natural policy gradient (NPG) method [Kakade, 2001]

For $t = 0, 1, \cdots$

$$\theta^{(t+1)} = \theta^{(t)} + \eta (\mathcal{F}_\rho^\theta)^\dagger \nabla_\theta V^{\pi_\theta^{(t)}}(\rho)$$

where η is the learning rate and $\mathcal{F}_\rho^\theta$ is the Fisher information matrix:

$$\mathcal{F}_\rho^\theta := \mathbb{E}\left[\big(\nabla_\theta \log \pi_\theta(a|s)\big) \big(\nabla_\theta \log \pi_\theta(a|s)\big)^\top \right].$$

Connection with TRPO/PPO

TRPO/PPO (Schulman et al., 2015; 2017) are popular heuristics in training RL algorithms, with **KL regularization**

$$\mathsf{KL}(\pi_\theta^{(t)} \| \pi_\theta) \approx \frac{1}{2}(\theta - \theta^{(t)})^\top \mathcal{F}_\rho^\theta (\theta - \theta^{(t)})$$

via constrained or proximal terms:

$$\begin{aligned}\theta^{(t+1)} &= \mathsf{argmax}_\theta V^{\pi_\theta^{(t)}}(\rho) + (\theta - \theta^{(t)})^\top \nabla_\theta V^{\pi_\theta^{(t)}}(\rho) - \eta \mathsf{KL}(\pi_\theta^{(t)} \| \pi_\theta) \\ &\approx \theta^{(t)} + \eta (\mathcal{F}_\rho^\theta)^\dagger \nabla_\theta V^{\pi_\theta^{(t)}}(\rho),\end{aligned}$$

leading to exactly NPG!

NPG $\approx$ TRPO/PPO!

NPG in the tabular setting

Natural policy gradient (NPG) method (Tabular setting)

For $t = 0, 1, \cdots$, NPG updates the policy via

$$\pi^{(t+1)}(\cdot|s) \propto \underbrace{\pi^{(t)}(\cdot|s)}_{\text{current policy}} \underbrace{\exp\left(\frac{\eta Q^{(t)}(s,\cdot)}{1-\gamma}\right)}_{\text{soft greedy}} \propto \pi^{(t)}(\cdot|s) \exp\left(\frac{\eta A^{(t)}(s,\cdot)}{1-\gamma}\right)$$

where $Q^{(t)} := Q^{\pi^{(t)}}$ and $A^{(t)} := A^{\pi^{(t)}}$ is the Q/advantage function of $\pi^{(t)}$, and $\eta > 0$ is the learning rate.

- the derivation is left as an exercise; see [Agarwal et al., 2019].
- invariant with the choice of ρ
- Reduces to policy iteration (PI) when $\eta = \infty$.

Global convergence of NPG

Theorem 4 ([Agarwal et al., 2021])

Set $\pi^{(0)}$ as a uniform policy. For all $t \geq 0$, we have

$$V^{(t)}(\rho) \geq V^{\star}(\rho) - \left(\frac{\log|\mathcal{A}|}{\eta} + \frac{1}{(1-\gamma)^2}\right)\frac{1}{t}.$$

Implication: set $\eta \geq (1-\gamma)^2 \log|\mathcal{A}|$, we find an ϵ-optimal policy within at most

$$\frac{2}{(1-\gamma)^2\epsilon} \text{ iterations.}$$

Global convergence at a sublinear rate independent of $|\mathcal{S}|$, $|\mathcal{A}|$!

Key ingredients of the proof

Lemma 5 (Performance difference lemma)

For all policies π, π' and distributions ρ over $\mathcal{S}$,

$$V^{\pi}(\rho) - V^{\pi'}(\rho) = \frac{1}{1-\gamma}\mathbb{E}_{s' \sim d_{\rho}^{\pi}}\mathbb{E}_{a' \sim \pi(\cdot|s')}\left[A^{\pi'}(s', a')\right].$$

- measures the performance difference for any pairs of policies

Lemma 6 (Policy improvement of NPG)

$$V^{(t+1)}(\rho) - V^{(t)}(\rho) \geq \frac{(1-\gamma)}{\eta}\mathbb{E}_{s \sim \rho} \log Z_t(s) \geq 0$$

where $Z_t(s) = \sum_a \pi^{(t)}(a|s) \exp\left(\eta A^{(t)}(s,a)/(1-\gamma)\right)$.

- monotonic performance improvement of NPG

Step 1: bounding the optimality gap

Denote $d^\star := d^\star_\rho$, and $\pi_s := \pi(\cdot|s)$. By the performance difference lemma,

$$
\begin{aligned}
&V^\star(\rho) - V^{(t)}(\rho) \\
&= \frac{1}{1-\gamma}\mathbb{E}_{s\sim d^\star} \sum_a \pi^\star(a|s) A^{(t)}(s,a) \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d^\star} \sum_a \pi^\star(a|s) \log \frac{\pi^{(t+1)}(a|s) Z_t(s)}{\pi^{(t)}(a|s)} \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d^\star} \left(\mathsf{KL}(\pi^\star_s \| \pi^{(t)}_s) - \mathsf{KL}(\pi^\star_s \| \pi^{(t+1)}_s) + \sum_a \pi^\star(a|s) \log Z_t(s) \right) \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d^\star} \Big(\mathsf{KL}(\pi^\star_s \| \pi^{(t)}_s) - \mathsf{KL}(\pi^\star_s \| \pi^{(t+1)}_s) + \log Z_t(s) \Big) .
\end{aligned}
$$

Step 2: telescoping

By the improvement lemma $V^{(t+1)}(\rho) \geq V^{(t)}(\rho)$,

$$\begin{aligned} V^{\star}(\rho) - V^{(T-1)}(\rho) &\leq \frac{1}{T}\sum_{t=0}^{T-1}\Big(V^{\star}(\rho) - V^{(t)}(\rho)\Big) \\ &= \frac{1}{\eta T}\sum_{t=0}^{T-1}\mathbb{E}_{s\sim d^{\star}}\Big(\mathsf{KL}(\pi_s^{\star}\|\pi_s^{(t)}) - \mathsf{KL}(\pi_s^{\star}\|\pi_s^{(t+1)}) + \log Z_t(s)\Big) \\ &\leq \frac{1}{\eta T}\mathbb{E}_{s\sim d^{\star}}\mathsf{KL}(\pi_s^{\star}\|\pi_s^{(0)}) + \frac{1}{\eta T}\sum_{t=0}^{T-1}\mathbb{E}_{s\sim d^{\star}}\log Z_t(s), \end{aligned}$$

where the second term is bounded by the policy improvement lemma

$$\begin{aligned} \frac{1}{\eta}\sum_{t=0}^{T-1}\mathbb{E}_{s\sim d^{\star}}\log Z_t(s) &\leq \frac{1}{1-\gamma}\sum_{t=0}^{T-1}\Big(V^{(t+1)}(d^{\star}) - V^{(t)}(d^{\star})\Big) \\ &\leq \frac{1}{1-\gamma}\Big(V^{(T)}(d^{\star}) - V^{(0)}(d^{\star})\Big) \end{aligned}$$

Step 3: finishing up

Putting the above together,

$$
\begin{aligned}
& V^\star(\rho) - V^{(T-1)}(\rho) \\
& \leq \frac{1}{\eta T}\mathbb{E}_{s\sim d^\star}\mathsf{KL}(\pi_s^\star \| \pi_s^{(0)}) + \frac{1}{(1-\gamma)T}\Big(V^{(T)}(d^\star) - V^{(0)}(d^\star)\Big) \\
& \leq \frac{\log|\mathcal{A}|}{\eta T} + \frac{1}{(1-\gamma)^2 T},
\end{aligned}
$$

where we used $\mathsf{KL}(\pi_s^\star \| \pi_s^{(0)}) \leq \log|\mathcal{A}|$ and $V \leq \frac{1}{1-\gamma}$.

Proof of Lemma 6

Proof of $\log Z_t(s) \geq 0$**:**

$$\begin{aligned}
\log Z_t(s) &= \log \sum_a \pi^{(t)}(a|s) \exp\Big(\eta A^{(t)}(s,a)/(1-\gamma)\Big) \\
&\geq \sum_a \pi^{(t)}(a|s) \log \exp\Big(\eta A^{(t)}(s,a)/(1-\gamma)\Big) \qquad \text{(Jensen's inequality)} \\
&= \frac{\eta}{1-\gamma} \sum_a \pi^{(t)}(a|s) A^{(t)}(s,a) \\
&= \frac{\eta}{1-\gamma} \sum_a \pi^{(t)}(a|s) (Q^{\pi^{(t)}}(s,a) - V^{\pi^{(t)}}(s)) \\
&= 0
\end{aligned}$$

Proof of Lemma 6

Bounding $V^{(t+1)}(\rho) - V^{(t)}(\rho)$: by the performance difference lemma,

$$
\begin{aligned}
V^{(t+1)}(\rho) - V^{(t)}(\rho) &= \frac{1}{1-\gamma}\mathbb{E}_{s\sim d_\rho^{(t+1)}} \sum_a \pi^{(t+1)}(a|s)A^{(t)}(s,a) \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d_\rho^{(t+1)}} \sum_a \pi^{(t+1)}(a|s)\log\frac{\pi^{(t+1)}(a|s)Z_t(s)}{\pi^{(t)}(a|s)} \\
&= \frac{1}{\eta}\mathbb{E}_{s\sim d_\rho^{(t+1)}} \mathsf{KL}(\pi^{(t+1)}(s)\|\pi^{(t)}(s)) + \frac{1}{\eta}\mathbb{E}_{s\sim d_\rho^{(t+1)}}\log Z_t(s) \\
&\geq \frac{(1-\gamma)}{\eta}\mathbb{E}_{s\sim\rho}\log Z_t(s),
\end{aligned}
$$

where we use $d_\rho^{(t+1)} \geq (1-\gamma)\rho$ and $\log Z_t(s) \geq 0$.

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